

Short Communications

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Note on the space group of dibenzyl disulphide. By B. VAN DIJK and G. J. VISSER, *Laboratorium voor Structuurchemie, Rijksuniversiteit Groningen, Bloemsingel 10, Groningen, The Netherlands*

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The space group of dibenzyl disulphide is $C2/c$.

The difficulties encountered by Lee & Bryant (1969) when refining the structure of dibenzyl disulphide in space group $C2/c$ are due to the fact that the molecules have been placed on the line $[0y0]$ rather than on the line $[0y\frac{1}{2}]$ which coincides with the twofold axis in $C2/c$. After we had changed the z coordinates by $\Delta z = +0.25$, rapid convergence was obtained in a least-squares refinement for space group $C2/c$ on the TR4 computer in Groningen. Use was made of a program working in block diagonal approximation, in the final cycles Lee & Bryant's (1969) weighting scheme was used. The index R decreased to 0.086 ($R = 0.104$ for a structure factor calculation on the TR4 based on the parameters and scattering factors from Lee & Bryant's paper, space group Cc). The final coordinates of the non-hydrogen atoms are given in Table 1. The hydrogen atoms were fixed at a distance of 1.08 Å from their respective carbon atoms and were given an isotropic temperature factor

$$\exp(-5.0 \sin^2 \theta / \lambda^2).$$

Table 1. Final coordinates and standard deviations as calculated by the least-squares program

	x	y	z
S(1)	0.0041 (1)	0.0111 (2)	0.3399 (1)
C(1)	0.1030 (3)	0.1625 (6)	0.3902 (4)
C(2)	0.2065 (3)	0.1038 (4)	0.3819 (4)
C(3)	0.2541 (3)	-0.0152 (5)	0.4611 (3)
C(4)	0.3500 (3)	-0.0646 (6)	0.4539 (4)
C(5)	0.4034 (3)	0.0058 (5)	0.3722 (4)

Table 1 (cont.)

	x	y	z
C(6)	0.3575 (3)	0.1214 (7)	0.2975 (4)
C(7)	0.2595 (3)	0.1724 (5)	0.3030 (3)

The lengths of the C-C bonds in the benzene ring vary from 1.351 to 1.407 Å. The variation in these bond lengths is three times as large as expected from the standard deviations calculated by the least-squares program used in Groningen. Therefore all standard deviations calculated by this least-squares program have been multiplied by three. The lengths of the bonds not belonging to the benzene rings are (for numbering see Lee & Bryant, 1969): S(1)-S(2) = 2.015 (± 0.003), S(1)-C(1) = 1.844 (± 0.012), C(1)-C(2) = 1.491 (± 0.015) Å. These values are almost identical with the average values given by Lee & Bryant (1969).

In view of the discussion given above we think that the space group of dibenzyl disulphide is $C2/c$. Also in an early paper by Egartner, Halla & Schacherl (1932) this space group has been adopted, as according to these authors dibenzyl disulphide does not show a piezoelectric effect.

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References

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 LEE, J. D. & BRYANT, M. W. R. (1969). *Acta Cryst.* B25, 2497.

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A further note on the space group of dibenzyl disulfide. By HOWARD EINSPAHR* and JERRY DONOHUE, *Department of Chemistry and Laboratory for Research on the Structure of Matter, University of Pennsylvania, Pennsylvania 19104, U.S.A.*

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In agreement with van Dijk & Visser we find that the space group of dibenzyl disulfide is $C2/c$, and not Cc , as reported by Lee & Bryant.

On the basis of a least-squares refinement in $C2/c$, van Dijk & Visser (1971) concluded that it is the correct space group

of dibenzyl disulfide, rather than Cc reported by Lee & Bryant (1969). Our own work on this problem was completed before we learned of the work of van Dijk & Visser, and we wish to report here the results of some calculations not made by them. Our least-squares results differ only negligibly from theirs, the small discrepancies probably

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